Carbon-Nanotube-Based Nanotechnology

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Carbon nanotubes are large linear fullerenes (close-caged molecules) made of sheets of carbon atoms arranged in six-folded hexagonal patterns. Since their discovery in 1991, nanotubes (rolled up sheets of carbon) have been vigorously investigated both theoretically and experimentally. The single-wall nanotubes are the strongest fibers known, and, depending on how the carbon sheet is rolled, a nanotube possesses unusual electronic properties. NASA's primary interest in nanotubes derives from three technologically interesting properties. First, single-wall nanotubes can be either metallic or semiconducting, thus providing the possibility of nanotube heterojunctions for nanoelectronic components in future ultrafast computers. Second, nanotubes are hollow, tubular, caged molecules that can serve as lightweight containers for packing and carrying hydrocarbon fuels on future space missions. Third, nanotubes have very good elasto-mechanical (strongest, yet highly flexible, tubular fiber known) properties that can be used in a lightweight, highly elastic, and very strong fibrous material for use in fabricating future spacecraft components.

At Ames Research Center, two-, three-, and four-terminal nanotube heterojunctions have been designed as a prototype of carbon-based nanoelectronic devices. Carbon atoms in a single nanotube are arranged in hexagonal arrays. However, by introducing topological defects such as pentagons and heptagons, it is possible to connect metal and semiconducting tubes into prototypes of carbon-based diodes and transistors. At Ames, the two-terminal heterojunctions have been modeled and observed in experiments that are done in collaboration with researchers at Stanford University. The three-terminal heterojunctions, however, will be necessary if any current-driven carbon-based logic device is to be realized in experiments. An example of the Ames carbon nanotube three-terminal "T" heterojunction is shown in the first figure, in which a semiconducting nanotube (red) serving as a gate can modulate the current flowing in a metallic nanotube (green) connecting external source and drain terminals. Three-terminal nanotube heterojunctions are computer-simulated models that are yet to be made in experiments. However, these quasi-two-dimensional (2-D) junctions could be the building blocks of nanoscale tunnel junctions in a 2-D network of nanoelectronic devices. The electronic transport through nanotubes, as interconnects and switching devices, in the form of current versus voltage relationship, is also calculated. These will help in guiding experimentalists toward better characterization of nanotubes and their electronic behavior.

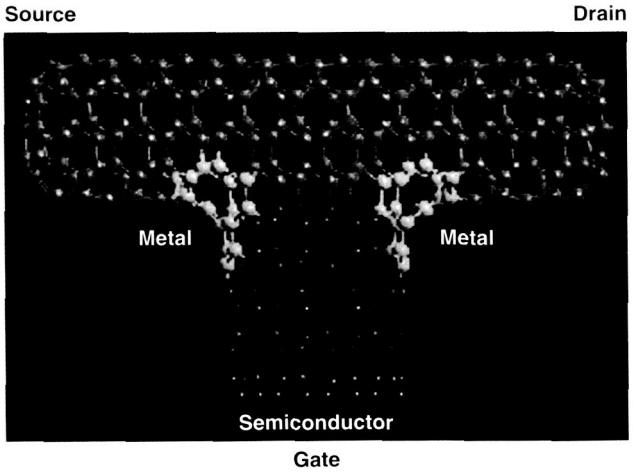

Fig. 1. Carbon-nanotube-based molecular electronics: carbon-nanotube three-terminal "T" heterojunction; red denotes semiconducting nanotube and green denotes metallic nanotube.

To exploit the elasto-mechanical properties of nanotubes, researchers at Ames Research Center and Stanford University have focused on using the nanotube as the tip in scanning-probe microscopes (SPM) to perform nanolithography on semiconductor surfaces. Simulations and experiments have shown that nanotubes are the smallest and strongest nanopencils that can read and write in nanoscale. Nanotube tips have enabled continuous lithography of 10 nanometer features, at a speed of up to 0.5 millimeters per second, over large silicon surface areas while simultaneously minimizing the tip-wear problem in conventional SPM-based nanolithography.

The search for low-cost, lightweight molecular hydrogen fuel storage and carrier material in solid booster rockets is crucial because of the potential it holds for effecting big reductions in overall system weight. Fullerenes, or nanotubes, are excellent candidates for they are lightweight, have large surface-to-volume ratios, and provide good adsorption characteristics for molecular hydrogen. Ames has shown in computer simulations that if nanotubes can be opened or closed in a controlled way, inner cavities of the nanotubes can be accessed for storing molecular hydrogen at higher pressures and densities than possible by any other means. The second figure shows that interstitial spacings in nanotube rope

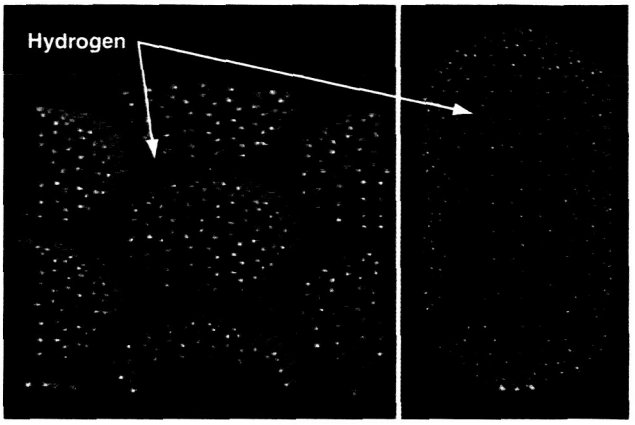

Fig. 2. Hydrogen storage in carbon nanotube: interstitial spacings in a carbon-nanotube rope; red denotes molecular hydrogen.

provide less volume to the stored hydrogen than storage within a closed-end nanotube. Computer simulations in conjunction with experimental efforts investigate the possibility of storing molecular hydrogen in nanotubes as nanoscale gas cylinders that can be carried on future space missions.

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Nanoelectronic Devices for the 21st Century

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Both physical and economic considerations indicate that the scaling era of complementary metal oxide semiconductor will run out of steam around the year 2010. However, physical laws also indicate that it is possible to compute at a rate of a billion times the present speeds with the expenditure of only 1 watt of electrical power. NASA has long-term goals for which ultrasmall semiconductor devices will be needed in critical applications: high-performance, low-power, compact computers for intelligent autonomous vehicles and petaflop (10^{15}) computing technology are two key examples.

Ames Research Center has developed a Green's-function-based code to calculate the transport properties of carbon nanotubes (CNTs). The single most important promise of CNTs with regard to device application is their use as quantum wires. An important question is how disorder affects the conductance of these low-dimensional systems. To obtain an understanding of this, both the low-bias conductance, as a function of the gate voltage (Fermi energy), and the conductance as a function of the applied bias in a CNT for two models of disorders, have been computed. These calculations show that in the presence of weak uniform disorder, the low-bias conductance exhibits a dip as the Fermi energy is swept across the intersection of the first and second sub-bands, as shown in the first figure; otherwise, the CNTs behave as a robust quantum wire. It was also